

Parity Nonconservation in Odd-isotopes of Single Trapped Atomic Ions

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We have estimated the size of the light-shifts due to parity nonconservation (PNC) interactions in different isotopes of Ba^+ and Ra^+ ions based on the work of Fortson [Phys. Rev. Lett. **70**, 2383 (1993)]. We have used the nuclear spin independent (NSI) amplitudes calculated earlier by us [Phys. Rev. Lett. **96**, 163003 (2006); Phys. Rev. A **78**, 050501(R) (2008)] and we have employed the third order many-body perturbation theory (MBPT(3)) in this work to estimate the nuclear spin dependent (NSD) amplitudes in these ions. Ra^+ is found to be more favourable than Ba^+ for measuring both the NSI and NSD PNC observables.

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Parity nonconservation (PNC) in an atom arises mainly due to the exchange of the Z^0 boson between the electrons and the nucleus [1]. The interaction leading to such an effect consists of two parts. One of them is nuclear spin-independent (NSI) and the other is nuclear spin-dependent (NSD). In addition, the interaction between the electrons and the nuclear anapole moment (NAM) in an atomic system which is NSD in character, can also give rise to PNC [1, 2]. Wood *et. al.* [2] have reported the observation of the NAM in atomic Cs. For an atomic system, the contribution of the NSI and NSD components can be extracted by using the addition and subtraction of two separate measurements respectively. However, it is not possible to distinguish the NSD contributions from the NAM or Z^0 exchange from these measurements, even though the latter is typically larger than the former in heavy atoms. Henceforth in this work, the term NSD interaction will refer to the combination of these two interactions.

Although Wood *et. al.* [2] claim to have observed the NAM in atomic Cs, it has so far not been possible to explain this observation from well established nuclear data [3]. Therefore, there is an urgent need to study the NSD part of atomic PNC. In atomic transitions when both the NSI and NSD interactions contribute simultaneously, the typical strength of the NSD component is much smaller than its NSI counterpart. The overall magnitudes of the both interactions grow rapidly with the atomic size [1]. It may therefore appear that heavier atomic systems would be a natural choice for studying the PNC transi-

tions. But in a certain cases, the PNC observables can also be enhanced due to degeneracies [4]. To date all the observations of atomic PNC have been reported in neutral systems [1]. However, Fortson in 1993 proposed that a single trapped and laser cooled ion can be used for measuring PNC with an accuracy that is comparable to that of their neutral counterparts [5]. This proposal is based on the interference of the PNC induced electric dipole amplitude ($E1_{PNC}$) with the electric quadrupole (E2) amplitude in the $6s\ ^2S_{1/2} \rightarrow 5d\ ^2D_{3/2}$ transition in Ba^+ which leads to a PNC induced light shift. This approach is being pursued at KVI [6, 7] in an experiment with the ion of the next heavier alkaline earth element Ra^+ , which has low-lying optical transitions. This effort has been preceded by many recent experimental and theoretical studies on properties related to PNC [6–12], and it appears that a high precision result for PNC in these ions is possible. In addition, a novel idea of observing only the NSD PNC interaction in the $S_{1/2} \rightarrow D_{5/2}$ transitions of these ions has been reported in Ref. [13].

In this paper, we compare the possible light-shifts due to PNC in the $^2S_{1/2} \rightarrow ^2D_{3/2}$ and $^2S_{1/2} \rightarrow ^2D_{5/2}$ transitions for Ba^+ and Ra^+ using our calculated results reported earlier [6, 10–12] as well as from this work. Only the NSD PNC amplitudes are evaluated here using the third order many-body perturbation theory (MBPT(3)). The results of these studies will aid in the choice of the hyperfine level transitions involving the $S_{1/2}$ and $D_{3/2,5/2}$ states in different isotopes for performing PNC experiments in order to extract the NSD PNC observables in a systematic and unambiguous way in the two above mentioned ions.

To measure the NSD PNC contribution, we propose to

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carry out measurements on $^{135,137}\text{Ba}$ ($I = 3/2$), ^{139}Ba ($I = 7/2$), ^{225}Ra ($I = 1/2$), ^{223}Ra ($I = 3/2$) and ^{229}Ra ($I = 5/2$). All these isotopes have long nuclear lifetimes except ^{229}Ra , where the measurements can be performed in an on-line facility.

In a single ion experiment, the observable is the PNC electric dipole transition induced ac-Stark shift *i.e.* the PNC light shift in the ground state Zeeman sub-levels when a laser drives a $E2$ transition between the ground state and a meta-stable state. Generalizing the expression given by Fortson [5], the measured PNC light shift in the $S_{1/2} \rightarrow D_{3/2,5/2}$ transitions in a single ion experiment will have a small shift due to PNC as

$$\Delta\omega_{m_F}^{PNC} \approx -\frac{Re\Sigma_{m_{F'}}(W_{m_F m_{F'}}^{PNC*} W_{m_F m_{F'}}^{Quad})}{\sqrt{\Sigma_{m_{F'}}|W_{m_F m_{F'}}^{Quad}|^2}}, \quad (1)$$

and a much larger shift due to the quadrupole coupling between the same two levels,

$$\Delta\omega_{m_F}^{Quad} \approx \frac{(\omega_0 - \omega)}{2} - \sqrt{\Sigma_{m_{F'}}|W_{m_F m_{F'}}^{Quad}|^2}, \quad (2)$$

for a given sub-level m_F of a hyperfine state of angular momentum F , where ω_0 and ω are the atomic and optical frequencies, respectively. The Rabi frequency for the PNC-induced-dipole transition is given by

$$W_{m_F m_{F'}}^{PNC} = -\frac{1}{2} \sum_i (E1_{PNC})_i^{m_F m_{F'}} \mathcal{E}_i(r=0), \quad (3)$$

and the Rabi frequency for the quadrupole transition is given by

$$W_{m_F m_{F'}}^{Quad} = -\frac{1}{2} \sum_{i,j} (E2)_{ij}^{m_F m_{F'}} \left[\frac{\partial \mathcal{E}_i(r)}{\partial x_j} \right]_{r=0}, \quad (4)$$

where \mathcal{E} is the applied electric field. We use atomic unit (au) through out this work unless mentioned explicitly.

To the best of our knowledge, the $E1_{PNC}$ amplitudes for the $S_{1/2} \rightarrow D_{3/2}$ transitions due to the NSD interaction for these ions have not been calculated so far. Preliminary calculations of these amplitudes for the $S_{1/2} \rightarrow D_{5/2}$ transitions are given in Ref. [13] using the relativistic configuration interaction (CI) method, but the expression used in that work for the NSD-interaction is not compatible with our analysis. In what follows, we employ a relativistic MBPT(3) method (as described below) here to evaluate these amplitudes in a systematic fashion for both the NSD PNC transition amplitudes.

The NSD part of the PNC interaction Hamiltonian is given by

$$H_{PNC}^{NSD} = \frac{G_F}{2\sqrt{2}} \mathcal{R}_a \vec{\alpha} \cdot \vec{\mathbf{I}} \rho_{nuc}(r), \quad (5)$$

where G_F is the Fermi constant, $\rho_{nuc}(r)$ is the nuclear potential, $\vec{\alpha}$ is the Dirac matrix, $\vec{\mathbf{I}}$ is the nuclear spin and

\mathcal{R}_a is a dimensionless constant which has information about NAM. The $E1_{PNC}$ amplitude due to this Hamiltonian can be written as

$$E1_{PNC} = \frac{\langle \Psi_i^{(0)} | D | \Psi_f^{(1)} \rangle + \langle \Psi_i^{(1)} | D | \Psi_f^{(0)} \rangle}{\sqrt{\langle \Psi_f^{(0)} | \Psi_f^{(0)} \rangle \langle \Psi_i^{(0)} | \Psi_i^{(0)} \rangle}}, \quad (6)$$

where the subscript 0 and 1 represent the atomic wavefunctions and their first order corrections due to H_{PNC}^{NSD} , i and f represent the valence orbitals in the initial and final states, respectively, and D is the electric dipole operator.

In the MBPT method, we define wave operators $\Omega_{v,0}$ and $\Omega_{v,1}$ to calculate the unperturbed ($|\Psi_v^{(0)}\rangle$) and perturbed ($|\Psi_v^{(1)}\rangle$) wavefunctions as

$$|\Psi_v^{(k)}\rangle = \Omega_{v,k} |\Phi_v\rangle \quad \text{and} \quad \Omega_{v,k} = \sum_{n=0}^{\infty} \Omega_{v,k}^{(n)} \quad (7)$$

where $|\Phi_v\rangle$ is the Dirac-Fock (DF) wavefunction obtained using the Dirac-Coulomb Hamiltonian.

We use the generalized Bloch equation given below to calculate the unperturbed wavefunctions in our MBPT formulation (for $n \geq 1$) [14]

$$[\Omega_{v,0}^{(n)}, H_0] = Q V_r \Omega_{v,0}^{(n-1)} P - \sum_{m=1}^{n-1} \Omega_{v,0}^{(n-m)} P V_r \Omega_{v,0}^{(m-1)} P, \quad (8)$$

where H_0 is the DF Hamiltonian, V_r is the residual Coulomb interaction, $\Omega_{v,0}^{(0)} = 1$ and P and Q are the projection operators in the model and orthogonal spaces, respectively; *i.e.*

$$P = |\Phi_v\rangle \langle \Phi_v| \quad \text{and} \quad Q = 1 - P. \quad (9)$$

Following the similar procedure (for $n \geq 1$), we get

$$\begin{aligned} [\Omega_{v,1}^{(n)}, H_0] = & Q H_{PNC}^{NSD} \Omega_{v,0}^{(n)} P + Q V_r \Omega_{v,1}^{(n-1)} P \\ & - \sum_{m=0}^n \Omega_{v,0}^{(n-m)} P H_{PNC}^{NSD} \Omega_{v,0}^{(m)} P \\ & - \sum_{m=0}^{n-1} \Omega_{v,1}^{(n-m-1)} P V_r \Omega_{v,0}^{(m)} P \\ & - \sum_{m=1}^{n-1} \Omega_{v,0}^{(n-m)} P V_r \Omega_{v,1}^{(m)} P, \end{aligned} \quad (10)$$

where $\Omega_{v,1}^{(0)} = Q H_{PNC}^{NSD} P$. For the MBPT(3) approximation, we consider terms up to $n = 2$ to evaluate $E1_{PNC}$ given by

$$E1_{PNC} = \frac{\langle \Phi_i | \Omega_{i,0}^\dagger D \Omega_{f,1} | \Phi_f \rangle + \langle \Phi_i | \Omega_{i,1}^\dagger D \Omega_{f,0} | \Phi_f \rangle}{norm} \quad (11)$$

with $norm = \sqrt{\langle \Phi_f | \Omega_{f,0}^\dagger \Omega_{f,0} | \Phi_f \rangle \langle \Phi_i | \Omega_{i,0}^\dagger \Omega_{i,0} | \Phi_i \rangle}$.

In the angular momentum relations, we express

$$\begin{aligned} E1_{PNC} &= \langle (J_i, I); F_i M_i | D_{eff}^1 + D_{eff}^2 | (J_f, I); F_f M_f \rangle \\ &= (-1)^{F_i - M_i} \begin{pmatrix} F_i & 1 & F_f \\ -M_i & q & M_f \end{pmatrix} \mathcal{M}, \end{aligned} \quad (12)$$

where F is the total angular momentum due to the electron angular momentum (J) and the nuclear spin (I) with its azimuthal component M . Here $q = -1, 0, 1$

depending upon the values of M_i and M_f . $\mathcal{M} = \langle (J_i, I); F_i | D_{eff}^1 + D_{eff}^2 | (J_f, I); F_f \rangle$ is the reduced matrix element of effective rank one operators with

$$D_{eff}^1 = \frac{\Omega_{i,0}^\dagger D \Omega_{f,1}}{norm} \quad \text{and} \quad D_{eff}^2 = \frac{\Omega_{i,1}^\dagger D \Omega_{f,0}}{norm}. \quad (13)$$

The above expression is non-zero for $F_i = F_f, F_f \pm 1$.

With the expansion $H_{PNC}^{NSD} = \sum_\mu (-1)^\mu I_\mu K^{-\mu}$, it gives

$$\langle (J_i, I); F_i | D_{eff}^1 | (J_f, I); F_f \rangle = \eta \sum_{j \neq i} (-1)^{j_i - j_f + 1} \begin{Bmatrix} F_f & F_i & 1 \\ J_j & J_f & I \end{Bmatrix} \begin{Bmatrix} I & I & 1 \\ J_j & J_i & F_i \end{Bmatrix} \frac{\langle J_f || D || J_j \rangle \langle J_j || K^1 || J_f \rangle}{\epsilon_i - \epsilon_j} \quad (14)$$

and

$$\langle (J_i, I); F_i | D_{eff}^2 | (J_f, I); F_f \rangle = \eta \sum_{j \neq f} (-1)^{F_i - F_f + 1} \begin{Bmatrix} F_f & F_i & 1 \\ J_i & J_j & I \end{Bmatrix} \begin{Bmatrix} I & I & 1 \\ J_j & J_f & F_f \end{Bmatrix} \frac{\langle J_f || K^1 || J_j \rangle \langle J_j || D || J_f \rangle}{\epsilon_f - \epsilon_j}, \quad (15)$$

where $\eta = \sqrt{I(I+1)(2I+1)(2F_i+1)(2F_f+1)}/norm$, ϵ_i represents orbital energy for i and the matrix element in terms of single particle orbitals is given by

$$\langle J_i || K^1 || J_f \rangle = i \frac{G_F}{2\sqrt{2}} \frac{\kappa_a}{I} \int_0^\infty dr \rho_{nuc}(r) [\langle \kappa_i || \sigma || -\kappa_f \rangle P_i(r) Q_f(r) - \langle -\kappa_i || \sigma || \kappa_f \rangle Q_i(r) P_f(r)], \quad (16)$$

for $P(r)$ and $Q(r)$ being the large and small radial components of Dirac wavefunction and σ is the Pauli spinor with $\langle \kappa_i || \sigma || \kappa_f \rangle = (\kappa_i + \kappa_f - 1) \langle \kappa_i || C^1 || \kappa_f \rangle$ for the Racah tensor C and the relativistic quantum number κ .

In the method proposed by Fortson, the PNC electric dipole transition induced light shift is observed as a frequency shift of the ground state Larmor frequency in spin zero isotopes. Any fluctuation of the quadrupole transition induced light shift does not modify the uncertainty of the PNC light shift measurement, since it cancels out in the Zeeman transition due to its m_F dependence (see Eqs. (1) and (2)). However, in the case of non-zero spin isotopes of these ions, the $\pm m_F$ transitions are forbidden by the $E2$ selection rules.

The estimated magnitudes of the PNC light shifts for both NSI and NSD in the $S_{1/2} \rightarrow D_{3/2,5/2}$ transitions are given in Table I (only non negligible values are given). For the calculations, we have used our earlier results for NSI PNC and electric quadrupole transition amplitudes [6, 10–12] and the NSD amplitudes have been evaluated in this work. On practical grounds, we have taken the strength of the electric field as 2×10^6 V/m; this value optimizes the quenching rate for Ba^+ , and $R_a \approx 0.2$, obtained from the Cs NSD PNC studies [2, 3].

It is clear from the above table, the NSD PNC light shift in the case of the $S_{1/2} \rightarrow D_{3/2}$ transition is about a few mHz (see Table I) which requires the measurement of the combined PNC light shift to less than 0.5%

precision. The allowed spin flip transitions in these isotopes are associated with not only the desired differential PNC light shift but also a much larger differential quadrupole light shift. Thus to achieve a precision below 0.5%, all the sources of temporal variation of the quadrupole light shift need to be stable with uncertainty well below a percent. Only in such cases the measurements of the quadrupole and PNC light shifts within a short time interval can provide NSD PNC light shifts with the desired accuracies. However, a suitable choice of the hyperfine states and the Zeeman sublevels allows to avoid the systematics from the quadrupole light shift. In the $F = 2(S_{1/2}) \rightarrow F' = 3(D_{3/2})$ transition in spin $I = 3/2$ isotopes, the sublevels $m_F = 1, 0$ of $F = 2(S_{1/2})$ will have the same quadrupole light shift and this will reduce the systematic error in the NSD PNC measurement. An unambiguous measurement of NSD PNC will indeed be a challenge, since it is necessary to know the NSI PNC part in the same isotope. An alternative is to consider the $F = 3(S_{1/2}) \rightarrow F' = 2(D_{3/2})$ transitions in $^{139}\text{Ba}^+$ ($I = 7/2$) and $^{229}\text{Ra}^+$ ($I = 5/2$). In these isotopes $m_F = 3, 1$ sublevels ($F = 3, S_{1/2}$) experience the same quadrupole light shift while $m_F = 2$ is free from the quadrupole and PNC light shifts. Thus it would be possible to extract both contributions to the PNC by driving the spin flip transitions after preparing the ion in the $m_F = 2$ state.

In principle an unambiguous measurement of NSD

TABLE I: Induced light-shifts due to E2 and PNC interactions in different isotopes of Ba⁺ and Ra⁺. $\mathcal{R}_a \approx 0.2$ from the Cs data [2, 3] and electric fields as 2×10^6 V/m are considered for the practical estimations.

Transition	$\langle j_i, 1/2 E1_{PNC}^{NSI} j_f, 1/2 \rangle$ ($\times 10^{-11} iea_0$) [6, 10]	$\langle j_i E2 j_f \rangle$ (au) [11, 12]	F_i	F_f	$\langle F_i E1_{PNC}^{NSD} F_f \rangle$ ($\times 10^{-14} iea_0 / \mathcal{R}_a$)	m_F	$\Delta\omega^{Quad}/2\pi$ (MHz)	$\Delta\omega_{PNC}^{NSI}/2\pi$ (Hz)	$\Delta\omega_{PNC}^{NSD}/2\pi$ ($\times 10^{-4}$ Hz)
^{135/137} Ba ⁺ ($I = 3/2$)									
6s \rightarrow 5d _{3/2}	2.46	12.74	2	3	97.18	1	7.62	-0.24	6.08
			1	2	-89.40	1	9.53	-0.37	-14.03
6s \rightarrow 5d _{5/2}	0	15.96	2	3	1.37	1	11.13	0	0.09
¹³⁹ Ba ⁺ ($I = 7/2$)									
6s \rightarrow 5d _{3/2}	2.46	12.74	3	3	103.57	1	5.07	0.42	12.29
			3	2	-105.55	3	3.6	-0.47	-14.75
						1	3.6	-0.1	2.95
6s \rightarrow 5d _{5/2}	0	15.96	3	2	0.608	3	12.87	0	0.08
						1	12.87	0	-0.02
²²⁵ Ra ⁺ ($I = 1/2$)									
7s \rightarrow 6d _{3/2}	46.4	-14.87	1	2	991.75	1	38.95	9.97	155.6
²²³ Ra ⁺ ($I = 3/2$)									
7s \rightarrow 6d _{3/2}	46.4	-14.87	2	3	1173.45	1	22.03	-4.7	73.35
			1	2	-1017.49	1	27.54	-7.05	-159.64
7s \rightarrow 6d _{5/2}	0	-19.04	2	3	-17.52	1	32.08	0	-1.1
²²⁹ Ra ⁺ ($I = 5/2$)									
7s \rightarrow 6d _{3/2}	46.4	-14.87	3	2	325.94	3	29.44	-4.19	45.56
						1	29.44	0.83	-9.11
			2	2	1147.73	1	17.42	7.42	152.18
7s \rightarrow 6d _{5/2}	0	-19.04	3	2	-5.12	3	17.5	0	-0.72
						1	17.5	0	0.14

PNC would be possible in the $S_{1/2} \rightarrow D_{5/2}$ transition, but the size of the observable light shift is very small; hence its realization is a challenge. In Table I the light shifts in the $S_{1/2} \rightarrow D_{5/2}$ transitions with different hyperfine states are given for various isotopes of these ions where it is feasible to drive spin flip transition between the magnetic sublevels avoiding the differential quadrupole light shift. It shows that an experimental uncertainty below 0.05% of the Larmor frequency shift measurement is essential to extract NAM result.

In conclusion, we have given the estimated values of the light shifts due to the nuclear spin independent and dependent parity nonconserving interactions for various isotopes of singly ionized barium and radium isotopes. We have shown that the size of these effects would be rather small for Ba⁺, and therefore it would be quite challenging to observe the nuclear spin dependent parity nonconserving effect in this ion. But in the case of Ra⁺, the prospects for observing the parity nonconserving light-shift due to the nuclear spin dependent interaction are much better. An unambiguous observation of light-shift due to nuclear spin-dependent interaction in the $7s \ ^2S_{1/2} \rightarrow 6d \ ^2D_{5/2}$ transition might be feasible in singly ionized radium. Our analysis highlights the isotopes of Ra⁺ and the transitions in them that could be suitable for observing the nuclear spin-dependent parity nonconservation.

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